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The (revised) Szeged index and the Wiener index of a nonbipartite graph

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Abstract

Hansen et. al. used the computer programm AutoGraphiX to study the differences between the Szeged index $Sz(G)$ and the Wiener index $W(G)$, and between the revised Szeged index $Sz^*(G)$ and the Wiener index for a connected graph G. They conjectured that for a connected nonbipartite graph G with $n \geq 5$ vertices and girth $g \geq 5$, $Sz(G) - W(G) \geq 2n - 5$. Moreover, the bound is best possible as shown by the graph composed of a cycle on 5 vertices, C_5, and a tree T on $n-4$ vertices sharing a single vertex. They also conjectured that for a connected nonbipartite graph G with $n \geq 4$ vertices, $Sz^*(G) - W(G) \geq \frac{n^2+4n-6}{4}$. Moreover, the bound is best possible as shown by the graph composed of a cycle on 3 vertices, C_3, and a tree T on $n-3$ vertices sharing a single vertex. In this paper, we not only give confirmative proofs to these two conjectures but also characterize those graphs that achieve the two lower bounds.

Keywords: Wiener index, Szeged index, revised Szeged index.

AMS subject classification 2010: 05C12, 05C35, 05C90, 92E10.

1 Introduction

All graphs considered in this paper are finite, undirected and simple. We refer the readers to [2] for terminology and notation. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V$, $d_G(u, v)$ denotes the *distance* between u and v min G. The *Wiener index* of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v).$$

This topological index has been extensively studied in the mathematical literature; see, e.g., [5, 7]. Let $e = uv$ be an edge of G, and define three sets as follows:

$$N_u(e) = \{w \in V : d_G(u, w) < d_G(v, w)\},$$

$$N_v(e) = \{w \in V : d_G(v,w) < d_G(u,w)\},$$
$$N_0(e) = \{w \in V : d_G(u,w) = d_G(v,w)\}.$$

Thus, $\{N_u(e), N_v(e), N_0(e)\}$ is a partition of the vertices of G respect to e. The number of vertices of $N_u(e)$, $N_v(e)$ and $N_0(e)$ are denoted by $n_u(e)$, $n_v(e)$ and $n_0(e)$, respectively. A long time known property of the Wiener index is the formula [6, 14]:

$$W(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e),$$

which is applicable for trees. Motivated the above formula, Gutman [4] introduced a graph invariant, named as the *Szeged index* as an extension of the Wiener index and defined by

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e).$$

Randić [12] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named as the *revised Szeged index*. The revised Szeged index of a connected graph G is defined as

$$Sz^*(G) = \sum_{e=uv\in E(G)} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right).$$

Some properties and applications of the Szeged index and the revised Szeged index have been reported in [1, 3, 9–11, 15].

We have known that for a connected graph, $Sz^*(G) \geq Sz(G) \geq W(G)$. It is easy to see that $Sz^*(G) = Sz(G) = W(G)$ if G is a tree, which means $m = n-1$. So we want to know the differences between $Sz(G)$ and $W(G)$, and between $Sz^*(G)$ and $W(G)$ for a connected graph with $m \geq n$.

In [8] Hansen et. al. used the computer programm AutoGraphiX and made the following conjectures:

Conjecture 1.1 *Let G be a connected bipartite graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz(G) - W(G) \geq 4n - 8.$$

Moreover, the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n-3$ vertices sharing a single vertex.

Conjecture 1.2 *Let G be a connected bipartite graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz^*(G) - W(G) \geq 4n - 8.$$

Moreover, the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n-3$ vertices sharing a single vertex.

Conjecture 1.3 *Let G be a connected graph with $n \geq 5$ vertices and girth $g \geq 5$ and with an odd cycle. Then*

$$Sz(G) - W(G) \geq 2n - 5.$$

Moreover, the bound is best possible as shown by the graph composed of a cycle on 5 vertices C_5 and a tree T on $n-4$ vertices sharing a single vertex.

Conjecture 1.4 *Let G be a connected graph with $n \geq 4$ vertices and $m \geq n$ edges and with an odd cycle. Then*

$$Sz^*(G) - W(G) \geq \frac{n^2 + 4n - 6}{4}.$$

Moreover, the bound is best possible as shown by the graph composed of a cycle on 3 vertices C_3 and a tree T on $n-3$ vertices sharing a single vertex.

In [3] we showed that both Conjecture 1.1 and 1.2 are true. In this paper, we will give confirmative proofs to Conjecture 1.3 and Conjecture 1.4. During the proof of Conjecture 1.3, we find another case which also makes the equality holds, that is the graph composed of a cycle on 5 vertices, C_5, and two trees with roots v_1, v_2 in C_5 satisfying $v_1v_2 \in E(C_5)$. So we get the following theorem:

Theorem 1.5 *Let G be a connected nonbipartite graph on $n \geq 5$ vertices and girth $g \geq 5$. Then*

$$Sz(G) - W(G) \geq 2n - 5.$$

Equality holds if and only if G is composed of a cycle C_5 on 5 vertices, and one tree rooted at a vertex of the cycle C_5 or two trees, respectively, rooted at two adjacent vertices of the cycle C_5.

We notice that the method used in the proof of Theorem 1.5 can also be used to prove the bipartite case, and therefore this gives another proof to Conjecture 1.1 other than that in [3].

2 Main results

We start this section with two definitions that are needed in our later proofs frequently.

Definition 1. Let P be a shortest path between two vertices x and y in a graph G, P' another path from x to y in G. We call P' the *second shortest path* between x and y, if $P' \neq P$, $|P'| - |P|$ is minimum, and if there are more than one path satisfying the condition, we choose P' as a one with the most common vertices with P in G.

Definition 2. A subgraph H of a graph G is called *isometric* if distance between any pair of vertices in H is the same as their distance in G.

In [13] Gutman gave another expression for the Szeged index:

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e) = \sum_{e=uv\in E(G)} \sum_{\{x,y\}\subseteq V(G)} \mu_{x,y}(e)$$

where $\mu_{x,y}(e)$, interpreted as contribution of the vertex pair x and y to the product $n_u(e)n_v(e)$, is defined as follows:

$$\mu_{x,y}(e) = \begin{cases} 1, & \text{if} \begin{cases} d_G(x,u) < d_G(x,v) \text{ and } d_G(y,v) < d_G(y,u), \\ \text{or} \\ d_G(x,v) < d_G(x,u) \text{ and } d_G(y,u) < d_G(y,v), \end{cases} \\ 0, & \text{otherwise.} \end{cases}$$

From above expressions, we know that

$$\begin{aligned} Sz(G) - W(G) &= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in E(G)} \mu_{x,y}(e) - \sum_{\{x,y\}\subseteq V(G)} d_G(x,y) \\ &= \sum_{\{x,y\}\subseteq V(G)} \left(\sum_{e\in E(G)} \mu_{x,y}(e) - d_G(x,y) \right). \end{aligned}$$

For convenience, let $\pi(x,y) = \sum_{e\in E(G)} \mu_{x,y}(e) - d_G(x,y)$.

Let G be a connected graph. For every pair $\{x,y\} \subseteq V(G)$, let P_1 be the shortest path between x and y. We know that for all $e \in E(P_1)$, $\mu_{x,y}(e) = 1$, which means that $\pi(x,y) \geq 0$. Let P_2 be the second shortest path between x and y (if there exists). Then $P_1 \Delta P_2 = C$, where C is a cycle. Let $P_i' = P_i \bigcap C = x'P_iy'$. If $E(P_1) \bigcap E(P_2) = \emptyset$, then $x' = x, y' = y$.

Now we have the following lemma.

Lemma 2.1 *For every pair $\{x,y\} \subseteq V(G)$, and C, x', y' defined as above,*
(1) if C is an even cycle, then $\pi(x,y) \geq d_C(x',y') \geq 1$;
(2) if C is an odd cycle and $d_C(x',y') \geq 2$, then $\pi(x,y) \geq 1$.

Proof. Firstly, we prove that for every $v \in V(C)$, $d_C(x',v) = d_G(x',v)$. If $v \in P_1'$, it is simply true; otherwise, we can find a shorter path between x' and y', and then we can find a shorter path between x and y. If $v \in P_2'$ and $d_C(x',v) > d_G(x',v) = |E(P_3)|$, where P_3 is a shortest path between x' and v in G, then the path $xP_2x'P_3vP_2y'P_2y$ between x and y is shorter than P_2, a contradiction. For the same reason, we have $d_C(y',v) = d_G(y',v)$ for all $v \in V(C)$. Similarly, it is easy to see that a shortest path from x (or y) to the vertex v in P_2' is $xP_2x'(yP_2y')$ together with a shortest path from $x'(y')$ to v in C. So, if an edge e in $E(C)$ makes $\mu_{x',y'}(e) = 1$, then we have $\mu_{x,y}(e) = 1$.

If C is an even cycle, we know that $|E(P_2')| \geq |E(P_1')|$. For every edge e in the antipodal edges of P_1' in C, it is obviously that $\mu_{x',y'}(e) = 1$, and then $\mu_{x,y}(e) = 1$. Hence, $\sum_{e \in E(G)} \mu_{x,y}(e) = d_G(x,y) + d_C(x',y')$, which means that $\pi(x,y) \geq d_C(x',y') \geq 1$.

If C is an odd cycle, there are vertices x_1, x_2, y_1, y_2 such that

$$d_C(x', x_1) = d_C(x', x_2), \tag{2.1}$$
$$d_C(y', y_1) = d_C(y', y_2). \tag{2.2}$$

Let $d_C(x_1, y_1) = min\{\ d_C(x_i, y_j), i, j \in \{1,2\}\}$. For every edge e in a shortest path between x_1 and y_1, we have $\mu_{x,y}(e) = \mu_{x',y'}(e) = 1$. So, $\sum_{e \in E(G)} \mu_{x,y}(e) \geq d_G(x,y) + d_C(x_1, y_1)$, which means that $\pi(x,y) \geq d_C(x_1, y_1)$.

Next we show that $d_C(x_1, y_1) \geq 1$. From equations 2.1 and 2.2, we have

$$d_C(x', x_1) = d_C(x', y') + d_C(y', x_1) - 1,$$

$$d_C(y', y_1) = d_C(x', y') + d_C(x', y_1) - 1.$$

If $d_C(x_1, y_1) = 0$, that is $x_1 = y_1$, then by adding the above two equations, we get

$$d_C(x', y') = 1,$$

which contradicts the assumption $d_C(x', y') \geq 2$.

∎

From the proof of Lemma 2.1, we also get the following lemma.

Lemma 2.2 *For every pair $\{x, y\} \subseteq V(C)$, where C is an isometric cycle,*
(1) if C is an even cycle, then $\pi(x,y) \geq d_C(x,y) \geq 1$;
(2) if C is an odd cycle and $d_C(x,y) \geq 2$, then $\pi(x,y) \geq 1$.

Now, we give a confirmative proof of Theorem 1.5.

Proof of Theorem 1.5: Let $C = v_1 v_2 \cdots v_k v_1$ be a shortest odd cycle of G with length k, where $k \geq g \geq 5$. It is obvious that C is an isometric cycle. We consider the pair $\{x, y\} \subseteq V(G)$.

Case 1. $\{x, y\} \subseteq V(C)$.

If $d_C(x,y) \geq 2$, then by Lemma 2.2 we have $\pi(x,y) \geq 1$. Otherwise, $\pi(x,y) \geq 0$. Therefore,

$$\sum_{\{x,y\} \subseteq V(C)} \pi(x,y) \geq \binom{k}{2} - k.$$

Case 2. $x \in V(C), y \in V(G) \backslash V(C)$.

We will prove that for every $y \in V(G)\backslash V(C)$, there exist two vertices x_1, x_2 in C such that $\pi(x_1, y) \geq 1$ and $\pi(x_2, y) \geq 1$.

Assume that v_i is the vertex on C such that $d_G(v_i, y) = min_{v\in V(C)} d_G(v, y)$, and P_1 is a shortest path between v_i and y. Let $|E(P_1)| = p_1$. It is obvious that P_1 does not contain any vertex in C.

Now we show that $\pi(v_{i+2}, y) \geq 1$. Since $P_2 = yP_1v_iv_{i+1}v_{i+2}$ is a path from y to v_{i+2}, $p_1 = d_G(v_i, y) \leq d_G(v_{i+2}, y) \leq p_1 + 2$.

Subcase 2.1. $d_G(v_{i+2}, y) = p_1 + 2$.

In this case, P_2 is a shortest path from y to v_{i+2}. Let P_3 be a second shortest path between y and v_{i+2}, $C_1 = P_2 \triangle P_3$, $C_1 \cap P_2 \cap P_3 = \{x', y'\}$. By Lemma 2.1, $\pi(v_{i+2}, y) \geq 1$ except for the case that C_1 is an odd cycle and $d_{C_1}(x', y') = 1$. In this case, the length of P_3 is $(p_1 + 2) + |C_1| - 2 = p_1 + |C_1|$, which is not less than $p_1 + k$. Consider the path $yP_1v_iv_{i-1}v_{i-2}\cdots v_{i+2}$. It is a path between y and v_{i+2}, and its length is $p_1 + (k - 2) < p_1 + k$, contrary to the choice of P_3.

Subcase 2.2. $p_1 \leq d_G(v_{i+2}, y) < p_1 + 2$.

Let P_2' be a shortest path from y to v_{i+2}, and P_3' a second shortest path between y and v_{i+2}. Let $C_1' = P_2' \triangle P_3'$, $C_1' \cap P_2' \cap P_3' = \{x', y'\}$. If $P_3' = P_2$, since $g \geq 5$ and $|E(P_2')| \geq |E(P_1)|$, then $d_{C_1'}(x', y') \geq 2$, and by Lemma 2.1 we have $\pi(v_{i+2}, y) \geq 1$. If $P_3' \neq P_2$, by Lemma 2.1, $\pi(v_{i+2}, y) \geq 1$ except for the case that C_1' is an odd cycle and $d_{C_1'}(x', y') = 1$. But, this case cannot happen because the length of P_3' is $|E(P_2')| + |C_1'| - 2 \geq p_1 + |C_1'| - 2 \geq p_1 + k - 2 \geq p_1 + 3$, which is larger than the length of P_2, contrary to the choice of P_3'.

No matter which cases happen, we always have $\pi(v_{i+2}, y) \geq 1$. Similarly, we have $\pi(v_{i-2}, y) \geq 1$. Because $k \geq 5$, v_{i-2} is different from v_{i+2}. For all the remaining vertices in C, $\pi(v_j, y) \geq 0$ for $j \neq i-2, i+2$. Then, for a fixed $y \in V(G)\backslash V(C)$, we get that $\sum_{x\in V(C)} \pi(x, y) \geq 2$. Therefore,

$$\sum_{x\in V(C), y\in V(G)\backslash V(C)} \pi(x, y) \geq 2(n - k).$$

Case 3. $x, y \in V(G)\backslash V(C)$.

In this case, $\pi(x, y) \geq 0$.

From above cases, we have

$$\begin{aligned}
& Sz(G)-W(G)\\
= & \sum_{\{x,y\}\subseteq V(G)} \pi(x,y)\\
= & \sum_{\{x,y\}\subseteq V(C)} \pi(x,y)+\sum_{\substack{x\in V(C)\\ y\in V(G)\setminus V(C)}} \pi(x,y)+\sum_{\{x,y\}\subseteq V(G)\setminus V(C)} \pi(x,y)\\
\geq & \binom{k}{2}-k+2(n-k)\\
= & 2n+\frac{1}{2}k(k-7)\\
\geq & 2n-5.
\end{aligned}$$

for $k\geq 5$.

From the above inequalities, we see that equality holds if and only if $k=g=5$, $\pi(x,y)=1$ for all the nonadjacent pairs $\{x,y\}$ in C, and there are exactly two vertices v_1, v_2 in C such that $\pi(v_1,y)=1, \pi(v_2,y)=1$ for all $y\in V(G)\setminus V(C)$, and $\pi(x,y)=0$ for every pair $\{x,y\}\subseteq V(G)\setminus V(C)$.

We first claim that if the equality holds, then G is unicyclic. Suppose that $\mathcal{C}$ is the set of all cycles except the shortest cycle C. Let C' is a shortest cycle of $\mathcal{C}$, then C' is an isometric cycle. If C' is an even cycle, and there exists a pair of vertices $\{x,y\}\subseteq V(C')\setminus V(C)$, then by Lemma 2.2, $\pi(x,y)\geq 1$, a contradiction. So there is only one vertex $x\in V(C')\setminus V(C)$. Let v_i, v_j be the neighbors of x in C'. Then v_ix, xv_j together with a shortest path between them in C is a cycle C'' different from C. Since the length of C is 5, $d(v_i,v_j)\leq 2$, and the length of C'' is at most 4, contrary to the assumption that $g\geq 5$.

If C' is an odd cycle, and there exists a pair of nonadjacent vertices $\{x,y\}\subseteq V(C')\setminus V(C)$. Then by Lemma 2.2, $\pi(x,y)\geq 1$, a contradiction. If there are only two adjacent vertices x,y on $V(C')\setminus V(C)$, and let v_i be the neighbor of x in C and v_j the neighbor of y in C, then v_ixyv_j together with a shortest path between them in C is a cycle C_1 different from C. Since the length of C is 5 and $g\geq 5$, $d(v_i,v_j)=2$. Then C_1 is an isometric cycle, and by Lemma 2.2, $\mu_{v_i,v_j}(xy)=1$, and so $\pi(v_i,v_j)\geq 2$, a contradiction. If there is only one vertex $x\in V(C')\setminus V(C)$, and let v_i, v_j be the neighbors of x in C', then v_ix, xv_j together with a shortest path between them in C is a cycle C_2 different from C. Since the length of C is 5, $d(v_i,v_j)\leq 2$, and the length of C_2 is at most 4, contrary to the assumption that $g\geq 5$.

So, we have that G is a unicyclic graph with the only cycle C of length 5. Let $C=v_1v_2\cdots v_5v_1$, T_i be the component of $E(G)\setminus E(C)$ that contains the vertex $v_i (1\leq i\leq 5)$.

If there are at least three nontrivial T_is, say T_i, T_j, T_k, then there is a pair of vertices, say $\{v_i, v_j\}$ which are not adjacent. Let $x\in V(T_i)\setminus\{v_i\}$, $y\in V(T_j)\setminus\{v_j\}$. Then

$\{x, y\} \subseteq V(G)\backslash V(C)$. Since $d_C(v_i, v_j) = 2$, by Lemma 2.1, $\pi(x, y) \geq 1$, a contradiction. Therefore, there are at most two nontrivial T_is, say T_i, T_j. If v_i, v_j are not adjacent, similarly we can find $\{x, y\} \subseteq V(G)\backslash V(C)$ satisfying $\pi(x, y) \geq 1$, a contradiction. Thus, v_i, v_j must be adjacent. In this case, for any $x \in V(T_i)\backslash\{v_i\}$, $y \in V(T_j)\backslash\{v_j\}$, $\pi(x, y) = 0$, and for any $x \in V(T_i)\backslash\{v_i\}$, $\pi(x, v_{i-2}) = 1$, $\pi(x, v_{i+2}) = 1$, and $\pi(x, v_k) = 0$ for $k \neq i, j$. $y \in V(T_j)\backslash\{v_j\}$ is similar to the x case. By calculation, we have $Sz(G) - W(G) = 2n - 5$. If there is only one nontrivial T_i, we also can calculate that G satisfies $Sz(G) - W(G) = 2n - 5$. ∎

Here we notice that by the above same way, we can give another proof to Conjecture 1.1, and get the following result:

Theorem 2.3 *Let G be a bipartite connected graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz(G) - W(G) \geq 4n - 8.$$

Equality holds if and only if G is composed of a cycle on 4 vertices C_4 and a tree T on $n - 3$ vertices sharing a single vertex.

Proof. Let C be a shortest cycle of G, and assume that $C = v_1 v_2 \cdots v_g v_1$. Simply, C is an isometric cycle. We consider the pair $\{x, y\} \subseteq V(G)$.

Case 1. $\{x, y\} \subseteq V(C)$.

By Lemma 2.2, $\pi(x, y) \geq d_C(x, y)$. Thus, if xy is an edge of G, then $\pi(x, y) \geq 1$. Otherwise, $\pi(x, y) \geq 2$. Therefore,

$$\sum_{\{x,y\} \subseteq V(C)} \pi(x, y) \geq g + 2\left(\binom{g}{2} - g\right).$$

Case 2. $x \in V(C), y \in V(G)\backslash V(C)$.

Assume that v_i is a vertex on C such that $d_G(v_i, y) = min_{v \in V(C)} d_G(v, y)$, and P_1 is a shortest path between v_i and y. Then P_1 does not contain any vertices on C; otherwise, if $v_j \in P_1$, then $d_G(v_j, y) < d_G(v_i, y)$, contrary to the choice of v_i.

If there is only one path between y and v_i, then $\pi(y, v_i) = 0$ and v_i is a cut vertex. For any other vertex v_j in C, the path from y to v_j must go through v_i, and thus, $\mu_{v_i, v_j}(e) = \mu_{y, v_j}(e)$ for $e \in E(C)$. From Lemma 2.2, we have that if $v_i v_j$ is an edge of C, then $\pi(y, v_j) \geq 1$. If $d_C(v_i, v_j) \geq 2$, then $\pi(y, v_j) \geq 2$. Therefore,

$$\sum_{x \in V(C)} \pi(x, y) \geq 2 + 2(g - 3) = 2g - 4 \geq g.$$

If there are at least two paths between y and v_i, then, since G is a bipartite graph, by Lemma 2.1 $\pi(y, v_i) \geq 1$. And for each $v_j \in V(C)\backslash\{v_i\}$, there are at least two paths

from y to v_j, so $\pi(y, v_j) \geq 1$. Therefore,

$$\sum_{x \in V(C)} \pi(x, y) \geq g.$$

Case 3. $x \in V(G)\backslash V(C), y \in V(G)\backslash V(C)$.

In this case, $\pi(x, y) \geq 0$.

From the above cases, we have

$$\begin{aligned}
& Sz(G) - W(G) \\
= & \sum_{\{x,y\} \subseteq V(G)} \pi(x, y) \\
= & \sum_{\{x,y\} \subseteq V(C)} \pi(x, y) + \sum_{\substack{x \in V(C) \\ y \in V(G)\backslash V(C)}} \pi(x, y) + \sum_{\{x,y\} \subseteq V(G)\backslash V(C)} \pi(x, y) \\
\geq & \; g + 2(\binom{g}{2} - g) + g(n - g) \\
= & \; g(n - 2) \\
\geq & \; 4n - 8.
\end{aligned}$$

From the above inequalities, one can see that if equality holds, then $g = 4$, and $\pi(x, y) = 1$ for all the adjacent pairs $\{x, y\} \subseteq V(C)$, $\pi(x, y) = 2$ for all the nonadjacent pairs $\{x, y\} \subseteq V(C)$ and $\pi(x, y) = 0$ for every pair $\{x, y\} \subseteq V(G)\backslash V(C)$.

Now we show that if equality holds, then G is a unicyclic graph. Suppose that $\mathcal{C}$ is the set of all cycles except the shortest cycle C. Let C' is a shortest cycle of $\mathcal{C}$. Then C' is an isometric cycle. Since G is bipartite, C' is an even cycle. If there exists a pair of vertices $\{x, y\} \subseteq V(C')\backslash V(C)$, then by Lemma 2.1, $\pi(x, y) = 1$, a contradiction. So there is only one vertex $x \in V(C')\backslash V(C)$. Let v_i, v_j be the neighbors of x in C'. Then $v_i x, x v_j$ together with a shortest path between them in C is a cycle C'' different from C. Since the length of C is 4, $d(v_i, v_j) = 2$, and the length of C'' is 4, $\mu_{v_i,v_j}(x v_i) = \mu_{v_i,v_j}(x v_j) = 1$. Thus, $\pi(v_i, v_j) \geq 4$, a contradiction. Therefore, G is unicyclic.

Let T_i be the component of $E(G)\backslash E(C)$ that contains the vertex $v_i (1 \leq i \leq 4)$.

If there are at least two nontrivial T_is, say T_i, T_j, and let $x \in V(T_i)\backslash\{v_i\}$, $y \in V(T_j)\backslash\{v_j\}$, then $\{x, y\} \subseteq V(G)\backslash V(C)$, and there are at least two paths between x and y. By Lemma 2.1, $\pi(x, y) \geq 1$, a contradiction. Therefore, there is only one nontrivial T_i. In this case, we can calculate that G satisfies $Sz(G) - W(G) = 4n - 8$. Hence, equality holds if and only if G is the graph composed of a cycle on 4 vertices, C_4, and a tree T on $n - 3$ vertices sharing a single vertex.

∎

Since for a bipartite graph, we have $Sz^*(G) = Sz(G)$, which immediately implies Conjecture 1.2.

Next, we give a proof to Conjecture 1.4. At first we need the following Lemmas.

Lemma 2.4 *([13]) For a connected graph G with at least two vertices,*

$$Sz(G) \geq W(G),$$

with equality if and only if each block of G is a complete graph.

Lemma 2.5 *Let G be a connected graph with $n \geq 4$ vertices and $m \geq n$ edges and with an odd cycle. Then for every vertex $u \in V(G)$, there exists an edge $e = v_1v_2 \in E(G)$ such that $u \in N_0(e)$, that is, $\sum_{e\in E(G)} n_0(e) \geq n$.*

Proof. Suppose that there is a vertex $u \in V(G)$ such that for every $e = xy \in E(G)$, we have $d_G(u,x) \neq d_G(u,y)$. Let $d = ecc(u)$, $N^i(u) = \{v \in V(G) | d_G(u,v) = i\}, 1 \leq i \leq d$. By the assumption, we know that there is no edge in $N^i(u)$ for every i, that is, $N^i(u)$ is an independent set. Set $X = \{u\} \bigcup \bigcup_{1\leq i\leq d, i \text{ is even}} N^i(u)$, $Y = \bigcup_{1\leq i\leq d, i \text{ is odd}} N^i(u)$. Then $G = G[X,Y]$ is a bipartite graph with partite sets X and Y. But, G is a connected graph with an odd cycle, a contradiction. Hence, for every vertex $u \in V(G)$, there exists an edge $e = v_1v_2 \in E(G)$ such that $u \in N_0(e)$, and so we have $\sum_{e\in E(G)} n_0(e) \geq n$.

∎

Now we turn to solving Conjecture 1.4 and get the following result:

Theorem 2.6 *Let G be a connected nonbipartite graph with $n \geq 4$ vertices. Then*

$$Sz^*(G) - W(G) \geq \frac{n^2 + 4n - 6}{4}.$$

Equality holds if and only if G is composed of a cycle on 3 vertices, C_3, and a tree T on $n-3$ vertices sharing a single vertex.

Proof. By using $n_u(e) + n_v(e) + n_0(e) = n$ for every $e \in E(G)$, we have

$$\begin{aligned}
& Sz^*(G) - W(G) \\
= \;& \sum_{e=uv\in E(G)} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right) - W(G) \\
= \;& \sum_{e=uv\in E(G)} n_u(e)n_v(e) + \sum_{e=uv\in E(G)} \left(\frac{n_0(e)}{2}(n - n_0(e)) + \frac{n_0^2(e)}{4}\right) - W(G) \\
= \;& Sz(G) - W(G) + \sum_{e=uv\in E(G)} \left(\frac{n_0(e)}{2}n - \frac{n_0^2(e)}{4}\right)
\end{aligned}$$

Let $n_0 = \sum_{e=uv\in E(G)} \left(\frac{n_0(e)}{2}n - \frac{n_0^2(e)}{4}\right)$. If there are two edges e', e'' such that $n_0(e') \geq n_0(e'')$, and put $n_0'(e') = n_0(e') + 1$, $n_0'(e'') = n_0(e'') - 1$, $n_0'(e) = n_0(e)$ for other edges, then

$$\begin{aligned}
& n_0' - n_0 \\
= & \sum_{e=uv\in E(G)} \left(\frac{n_0'(e)}{2}n - \frac{n_0'^2(e)}{4}\right) - \sum_{e=uv\in E(G)} \left(\frac{n_0(e)}{2}n - \frac{n_0^2(e)}{4}\right) \\
= & \frac{n_0(e'') - n_0(e') - 1}{2} \\
< & \ 0.
\end{aligned}$$

Let C be a shortest odd cycle of G with length g, and its edges be $e_1, e_2, \cdots, e_g$. Then C is isometric. For every edge $e = uv \in E(C)$, there is a vertex $x \in V(C)$ such that $d_G(x,u) = d_C(x,u) = d_C(x,v) = d_G(x,v)$. Therefore, $n_0(e) \geq 1$ for every $e \in E(C)$. If there are two edges e', e'' such that $n_0(e') \geq n_0(e'')$, we could do the operation as above, which makes n_0 smaller. Thus, n_0 attains its minimum when $n_0(e_i) = 1$ except for $n_0(e_1)$, $n_0(e) = 0$ for all the remaining edges. By Lemma 2.5, $\sum_{e\in E(G)} n_0(e) \geq n$, and so $n_0(e_1) \geq n - g + 1$. Hence,

$$n_0 \geq (g-1)(\frac{n}{2} - \frac{1}{4}) + \frac{n-g+1}{2}n - \frac{(n-g+1)^2}{4} \geq \frac{n^2}{2} - \frac{1}{4}\left(2 + (n-2)^2\right) = \frac{n^2+4n-6}{4}.$$

From the above inequalities, we can see that equality holds if and only if $g = 3$, $Sz(G) = W(G)$ and $n_0(e_1) = n-2, n_0(e_2) = 1, n_0(e_3) = 1, n_0(e) = 0$ for all the remaining edges.

Now we conclude that G is unicyclic. Suppose that G is not unicyclic. By Lemma 2.4, we know there is a block H different from C which is a complete graph of order at least three. Then, $n_0(e) \geq 1$ for every $e \in E(H)$, a contradiction.

Let T_i be the component of $E(G)\backslash E(C)$ that contains the vertex $v_i (1 \leq i \leq 3)$.

If there are at least two nontrivial T_is, say T_1, T_2, then $n_0(v_2v_3) = |V(T_1)| \geq 2, n_0(v_1v_3) = |V(T_2)| \geq 2$, a contradiction. Therefore, there is only one nontrivial T_i. In this case, we can calculate that G satisfies $Sz^*(G) - W(G) = \frac{n^2+4n-6}{4}$. Hence, equality holds if and only if G is the graph composed of a cycle on 3 vertices, C_3, and a tree T on $n-3$ vertices sharing a single vertex. ∎

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